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On occurrence of spectral edges for periodic operators inside the Brillouin zone

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Abstract. The article discusses the following frequently arising question on the spectral structure of periodic operators of mathematical physics (e.g., Schrödinger, Maxwell, waveguide operators, etc.). Is it true that one can obtain the correct spectrum by using the values of the quasimomentum running over the boundary of the (reduced) Brillouin zone only, rather than the whole zone? Or, do the edges of the spectrum occur necessarily at the set of "corner" high symmetry points? This is known to be true in $1D$, while no apparent reasons exist for this to be happening in higher dimensions. In many practical cases, though, this appears to be correct, which sometimes leads to the claims that this is always true. There seems to be no definite answer in the literature, and one encounters different opinions about this problem in the community.

In this paper, starting with simple discrete graph operators, we construct a variety of convincing multiply-periodic examples showing that the spectral edges might occur deeply inside the Brillouin zone. On the other hand, it is also shown that in a "generic" case, the situation of spectral edges appearing at high symmetry points is stable under small perturbations. This explains to some degree why in many (maybe even most) practical cases the statement still holds.

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1. Introduction

The article discusses the following frequently arising question on the spectral structure of periodic operators of mathematical physics, which in particular is prominent due to the recent surge in studying photonic crystals [19]-[21], [36]-[38]. Let us have a periodic elliptic self-adjoint operator $L(x, D)$ (e.g., Schrödinger, Maxwell), where we use the standard notation $D = \frac{1}{i}\nabla$. The operator is considered in the whole space $\mathbb{R}^n$, or in a periodic domain (on a periodic periodic manifold), e.g. in a periodic waveguide. The standard Floquet-Bloch theory (e.g., [1, 35, 53]) shows that the spectrum of L in the infinite periodic medium can be obtained as follows: one fixes a value k of the quasimomentum in the first Brillouin zone B, finds the (discrete) spectrum of the corresponding Bloch Hamiltonian $L(k) = L(x, D + k)$ acting on periodic functions, and then takes the union over all quasimomenta in the Brillouin zone. The question we address in this work is whether the correct spectrum can be obtained as the union over the boundary of the Brillouin zone only‡

This is well known to be true in $1D$ (e.g., [13, 53]). In particular, the edges of the spectrum occur at the spectra of the periodic and anti-periodic problems on the single period. If this claim is correct in higher dimensions, the computational task is significantly simplified, due to reduced dimension. This is important, for instance, in optimization procedures, when one needs to run the spectral computation at each iteration [9, 10]. An experimental observation is that in most practical cases this is correct. One frequently encounters the belief that this is always true (albeit no justification is ever provided). On the other hand, unlike in $1D$, there is no analytic reason for this property to hold. Moreover, many researchers are aware that numerics sometimes produces counterexamples. Surprisingly, such examples are hard to come by and are usually not very convincing for an analyst (e.g., the error in computing the spectrum using only the boundary of the Brillouin zone is usually very small). The experience is that one needs to make the medium inside the fundamental domain (Wiegner-Seitz cell) truly asymmetric to achieve such examples.

The first goal of this text is to provide simple definite examples to disprove the claim that the edges of the spectral bands can be found by using the boundary of the (reduced) Brillouin zone only. This is done by first analyzing some discrete graph systems. Section 2 describes such combinatorial graph counterexamples. Section 3 deduces from this some quantum graph (see [39]) examples. Then in Section 4, we bootstrap this to examples of waveguide systems or Laplace-Beltrami operators on thin tubular branching manifolds. Possibilities for obtaining counterexamples of the Schrödinger and Maxwell cases are discussed in Section 5.

‡ If additional symmetries are present in the system, one considers the reduced (with respect to these symmetries) Brillouin zone. Another version of this question is whether the edges of the spectrum are attained on the set of high symmetry points of the Brillouin zone only. The importance of such points has been known since at least the paper [4]. When one needs to find the density of states, the full Brillouin zone is always required.

It is surprising, however, that the claim that we show to be incorrect in general, is still correct (or almost correct) so often. Thus, in many practical cases, computations along the boundary of the (reduced) Brillouin zone (and as a matter of fact, often at high symmetry corner points only) provide the correct spectrum. We suggest an explanation of this effect in the final Section 6. There we attempt to explain how it can happen that one often sees the spectral edges occurring at the high symmetry points only. It is shown that "generically" this occurrence is stable under small perturbations. In other words, there are open sets of "good" and "bad" periodic operators, the boundary between which consists of non-generic operators. This probably explains the frequent occurrence of the effect in practice.

Finally, the last sections provide additional remarks and acknowledgments.

2. Combinatorial graph examples

We start by considering difference operators acting on a periodic graph. These will serve to illustrate the general ideas in a situation which is not difficult to analyze. Furthermore, building upon them, we will provide examples of more complex periodic spectral problems with the desired spectral feature.

2.1. The main graph operators

We consider the $\mathbb{Z}^2$-periodic planar graph Γ, with the fundamental domain W shown in Figure 1 below. One imagines the graph Γ as obtained by tiling the plane with the

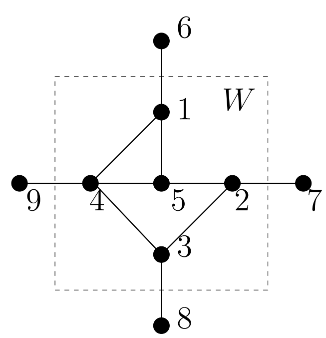

Figure 1. The graph Γ with fundamental region W.

$\mathbb{Z}^2$-shifted copies of W. We will label the vertices in W and near W with the numbers shown in Figure 1.

Let $\ell^2(\Gamma)$ be the Hilbert space of square-summable functions defined on the set of vertices of Γ. The discrete Laplacian on Γ can be defined in several (not always equivalent) ways (e.g., [6, 7]). We will use two of these.

The first one, Δ, is defined for $f \in \ell^2(\Gamma)$ by

$$(\Delta f)(v) := \sum_{u \sim v} f(u), \tag{2.1}$$

where the notation $u \sim v$ means that vertex u is adjacent (connected by an edge) to vertex v. For instance,

$$(\Delta f)(5) = f(1) + f(2) + f(4).$$

The Laplacian defined in (2.1) differs from another discrete Laplacian often used in the literature by the term $d_v f(v)$, where d_v is the degree (valence) of the vertex v: $\sum_{u\sim v} f(u) - d_v f(v)$.

We will also employ another version, L, of the Laplacian, which is defined as

$$(Lf)(v) := \frac{1}{\sqrt{d_v}} \sum_{u\sim v} \frac{1}{\sqrt{d_u}} f(u). \tag{2.2}$$

One could call it the Laplace-Beltrami operator. The need for this operator in our study will become clear when we move to the quantum graph case.

One notices that both Δ and L are bounded operators in $\ell^2(\Gamma)$.

In the case of a regular graph (i.e. the one with constant degrees $d_v = d$ of vertices), the spectra of Δ and L can be easily related. However, our graph Γ is not regular, and thus these spectra need to be studied independently.

The following statement is well known (e.g., [6]) and immediate:

Lemma 2.1. *The operators Δ and L commute with any automorphism $T \in \mathrm{Aut}(\Gamma)$ of the graph Γ. In particular, they commute with $\mathbb{Z}^2$-shifts on Γ.*

For $p = (p_1, p_2) \in \mathbb{Z}^2$, we denote by $T(p)$ the shift operator by p on Γ. E.g., $T(1,0)$ shifts the vertex 4 to the vertex 7 and $T(0,1)$ shifts 3 to 6.

Due to the periodicity of the operators, one can use the standard Floquet-Bloch theory [1, 13, 35, 53] to study their spectra. In the particular case of graphs, this theory is also described, for instance, in [16], [34]-[40], [49].

Let $k = (k_1, k_2)$ be a *quasimomentum* in the *Brillouin zone* $B = [-\pi, \pi]^2$. Consider the space ℓ^2_k of all functions f satisfying the following *Floquet (Bloch, cyclic) condition*:

$$f(T(p)v) = \mathrm{e}^{\mathrm{i}p\cdot k} f(v) \tag{2.3}$$

for all $p \in \mathbb{Z}^2$. Here $p \cdot k = p_1k_1 + p_2k_2$. Such a function f is clearly uniquely determined by the vector $(f_1, f_2, ..., f_5)^t$ of its values at the five vertices in W, and thus ℓ^2_k is five-dimensional and naturally isomorphic to $\ell^2(W)$.

Definition 2.2. *We will denote by Ξ the boundary ∂B of the Brillouin zone $B = [-\pi, \pi]^2$ and by X the set of points $k = (k_1, k_2) \in B$ such that k_1 and k_2 are integer multiples of π.*

We now define the Floquet Laplacian $\Delta(k) : \ell^2(W) \to \ell^2(W)$ as the restriction to the space ℓ^2_k of the operator Δ defined as in (2.1). In terms of the basis of the delta functions at vertices of W, this operator has the following matrix:

$$\Delta(k) := \begin{pmatrix} 0 & 0 & \mathrm{e}^{\mathrm{i}k_1} & 1 & 1 \\ 0 & 0 & 1 & \mathrm{e}^{\mathrm{i}k_2} & 1 \\ \mathrm{e}^{-\mathrm{i}k_1} & 1 & 0 & 1 & 0 \\ 1 & \mathrm{e}^{-\mathrm{i}k_2} & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \end{pmatrix}. \tag{2.4}$$

In a similar way, one can define $L(k)$ and observe that

$$L(k) = S^{-1}\Delta(k)S^{-1}, \tag{2.5}$$

where S is the matrix

$$S := \begin{pmatrix} \sqrt{3} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{3} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{3} \end{pmatrix}. \tag{2.6}$$

We now state the standard conclusion of the Floquet theory about the relation between the spectra of Δ and $\Delta(k)$, or L and $L(k)$ (e.g., [13, 16, 34, 35, 40, 49, 53]). For each fixed k, the matrix $\Delta(k)$ (correspondingly, $L(k)$) is self-adjoint, and thus admits a spectrum of 5 eigenvalues $\{\lambda_j(k)\}_{j=1}^5$ (correspondingly, $\{\mu_j(k)\}_{j=1}^5$), which we number in non-decreasing order. It is well known that then each of the functions $\lambda_j(k)$ is continuous. The multiple-valued function $k \mapsto \{\lambda_j(k)\}$ is called the *dispersion relation*. Its graph is the *dispersion curve*, also called the *Bloch variety*. Each of the individual functions $k \mapsto \lambda_j(k)$ is called the jth *branch* of the dispersion relation.

Proposition 2.3. *[13, 35, 34, 40, 53] The spectrum of Δ (correspondingly, L) is the union over $k \in B$ of the spectra of $\Delta(k)$ (correspondingly, $L(k)$):*

$$\begin{aligned} \sigma(\Delta) &= \bigcup_{k\in B} \sigma(\Delta(k)) = \bigcup_{k\in B}\bigcup_{j=1}^{5} \lambda_j(k), \\ \sigma(L) &= \bigcup_{k\in B} \sigma(L(k)) = \bigcup_{k\in B}\bigcup_{j=1}^{5} \mu_j(k). \end{aligned} \tag{2.7}$$

The segments $I_j = \bigcup\limits_{k\in B} \lambda_j(k)$ (and their analogs for the operator L) are called bands *of the spectrum of Δ (correspondingly, of L).*

Notice that our graph Γ does not have any point symmetries, and thus the reduced Brillouin zone is equal to the full one. So, the question we would like to address is whether one can replace the union over $k \in B$ in (2.7) by the union along the boundary $\Xi = \partial B$ of the Brillouin zone B only. A more restricted question is whether the band edges are attained at points of X only. As we will show in the next sub-section, both of these properties do not hold, and calculations along the boundary lead to significant errors in spectra of Δ and L.

2.2. Spectral edges - counterexamples

In this sub-section we show that computations along $\Xi = \partial B$ (and thus over X as well) do not necessarily lead to the correct spectra of Δ and L, and the errors can be significant. We are interested in whether the segments $I_j = \bigcup_{k\in B} \lambda_j(k)$ and $I'_j = \bigcup_{k\in\partial B} \lambda_j(k)$ coincide. We will show that for our examples, even the unions

$\sigma(\Delta) = \bigcup_{j=1}^{5} I_j$ and $\bigcup_{j=1}^{5} I'_j$ are different (the situation is analogous for L). This means that using only the boundary of the Brillouin zone, one does not recover the spectral edges (and thus the spectrum) correctly.

2.2.1. Operator Δ One can easily find the spectrum of the Floquet Laplacian $\Delta(k)$ (which is a simple 5×5 matrix), using for instance Matlab. Computing it for a grid in the Brillouin zone (we have used the uniform 64×64 grid in B), one can obtain the whole spectrum of Δ. This leads to the following numerical values of the five bands: $[-2.73, -1.90]$, $[-1.63, -1.00]$, $[-0.73, 0.73]$, $[0, 1.46]$, and $[2.00, 3.23]$. One notices that there are spectral gaps present between all consecutive bands, except the 3rd and 4th ones, which overlap.

Since it is sufficient for our purpose to provide a single counterexample, we will focus on the second band $[-1.63, -1.00]$ only.

A gray scale plot of the second branch (corresponding to the second band of the spectrum) is given in Figure 2 §. This numerical evidence shows that the band edges

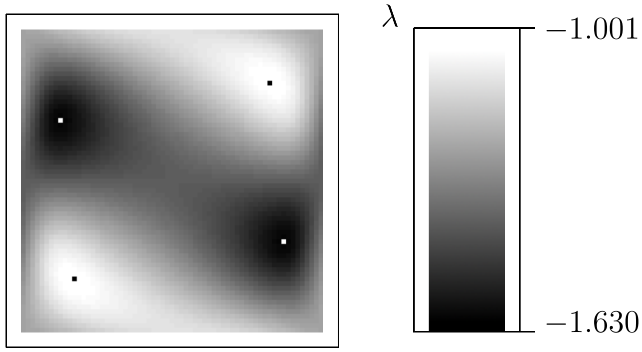

Figure 2. A gray scale image of the second branch of the spectrum of $\Delta(k)$. Extrema points are highlighted.

(i.e., the extrema of the branch function) occur at some values k not in Ξ. This is confirmed by the graph of the branch presented in Figure 3. Let us now make this observation rigorous by finding the maximum and minimum values of λ on Ξ. The characteristic polynomial of $\Delta(k)$ is

$$\begin{aligned} c_\Delta(\lambda; k) = \lambda^5 - 8\lambda^3 - (2\cos k_1 + 4\cos k_2 + 2)\lambda^2 \\ +(8 - 2\cos(k_1 + k_2) - 4\cos k_1 - 2\cos k_2)\lambda \\ -2\cos(k_1 + k_2) - 2\cos(k_1 - k_2) + 4\cos k_2. \end{aligned} \tag{2.8}$$

Since the second band does not intersect any others, standard perturbation theory [32] implies that the corresponding eigenvalue branch $\lambda(k) = \lambda_2(k)$ is analytic. It is not hard

§ This and other plots are drawn over the square $[0, 2\pi]^2$, rather than the Brillouin zone $B = [-\pi, \pi]^2$. The origin $(0, 0)$ is located in the upper left corner.

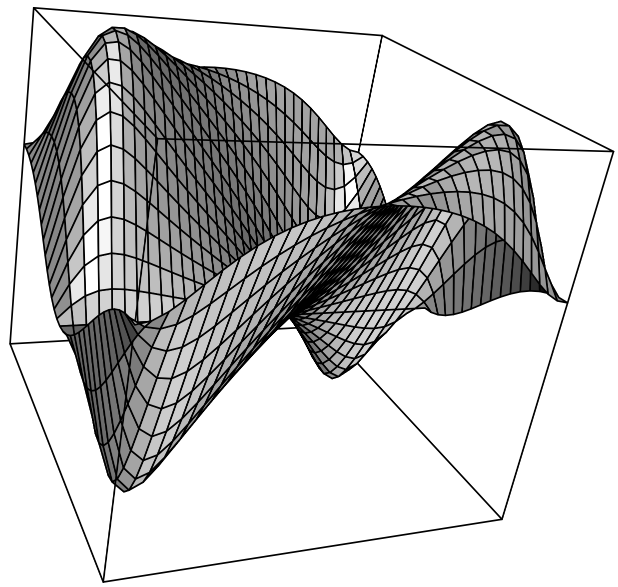

Figure 3. A graph of the second branch for the graph Γ.

to check all possible extremal values of λ on Ξ. Indeed, assuming that k_1 equals $\pm\pi$ or 0, one can differentiate the secular equation $c_\Delta(\lambda; k) = 0$ with respect to k_2 and use that at an extremal point (unless it is one of the points of X), one has $\frac{\partial\lambda}{\partial k_2} = 0$. One can do the same with the roles of k_1 and k_2 reversed. This calculation shows that extremal points can be located only where k_1 and k_2 are integer multiples of π, i.e. at X. All points of X can be checked to yield that the minimum value on X is $-\sqrt{2} \approx -1.414$, attained at $k = (\pi, 0)$ and $k = (\pi, \pi)$, and the maximum value is $-\sqrt{4 - \sqrt{8}} \approx -1.082$ at $k = (0, \pi)$. These values can be compared with the numerically found extreme values of -1.630 at $k \approx (1.865, 0.785)$ and -1.001 at $k \approx (-1.080, 5.203)$. This gives a difference of about 8% at the upper edge, and 15% at the lower edge. These values and their symmetric counterparts are highlighted in Figure 2.

In fact, the location and value of the maximum of the second branch can be found exactly. It is not hard to check that the value $\lambda = -1$ attained at $k_* = \left(\dfrac{\pi}{3}, \dfrac{5\pi}{3}\right)$ is a maximum.

Thus, we have an example of the situation when restricting the search of the edges of the spectrum to quasimomenta from Ξ, leads to significant errors.

One can draw other branches of the dispersion relation. They show that some of the branches do attain their extrema on X only, while some others do not.

2.2.2. Operator L The operator L can be analyzed similarly. We briefly summarize the findings. The characteristic polynomial for $L(k)$ is

$$\begin{aligned} c_L(\lambda;k) = \lambda^5 - \frac{7}{9}\lambda^3 - \left(\frac{1}{18} + \frac{1}{9}\cos k_2 + \frac{1}{18}\cos k_1\right)\lambda^2 \\ + \left(\frac{13}{162} - \frac{7}{162}\cos k_1 - \frac{1}{54}\cos k_2 - \frac{1}{54}\cos(k_1+k_2)\right)\lambda \\ + \frac{1}{81}\cos k_2 - \frac{1}{162}\cos(k_1-k_2) - \frac{1}{162}\cos(k_1+k_2). \end{aligned} \tag{2.9}$$

We observe that (2.9) is quite similar to (2.8), modulo changes in some constants. The structure of the branches of solutions to $c_L(\lambda; k) = 0$ are also qualitatively similar to the ones for the spectrum of Δ. The spectrum of L on Γ consists of five bands: $[-0.830, -0.606]$, $[-0.518, -0.297]$, $[-0.219, 0.219]$, $[0, 0.485]$, $[0.611, 1.000]$, with the third and fourth bands overlapping. The second branch is similar in appearance to the one of the operator Δ (see Figure 4). It shares the property that the band edges occur away from the set Ξ.

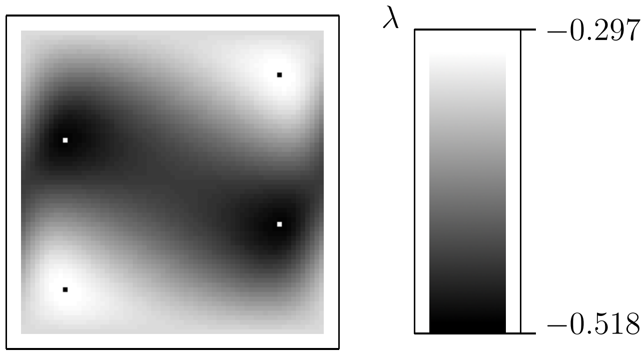

Figure 4. A gray scale image of the second branch for the operator L. Extrema are highlighted.

Analogously to the case of the operator Δ, we again find that the extremal values on Ξ of the second band function can only occur at the points $k \in X$. It turns out that the maximum value on Ξ is $-1/3 \approx -0.333$ at $k = (0, 0)$ and $k = (0, \pi)$, and the minimum value is $-\sqrt{2}/3 \approx -0.471$ at $k = (\pi, 0)$ and $k = (\pi, \pi)$. These can be compared with the numerically found maximum over all of B of approximately -0.297 at $k \approx (5.40, 0.88)$ and -0.518 at $k \approx (0.26, 0.88)$. The difference is 10.8% at the upper edge, and 9.5% at the lower edge.

In summary, we have described two difference operators Δ and L acting on a periodic graph Γ, which have spectra with band edges occurring away from the boundary of the Brillouin zone.

2.3. An example in the presence of point symmetries

The previously described examples dealt with a graph Γ that had only translation invariance with respect to $\mathbb{Z}^2$, and no point symmetries (i.e., symmetries that would fix a point on the graph). Thus, the Brillouin zone was not reduced. In this section, we provide an example where the point symmetry group is non-trivial, while the effect we observed in the previous sections still holds. We will also observe in some cases that spectral edges can occur on Ξ, but not on X.

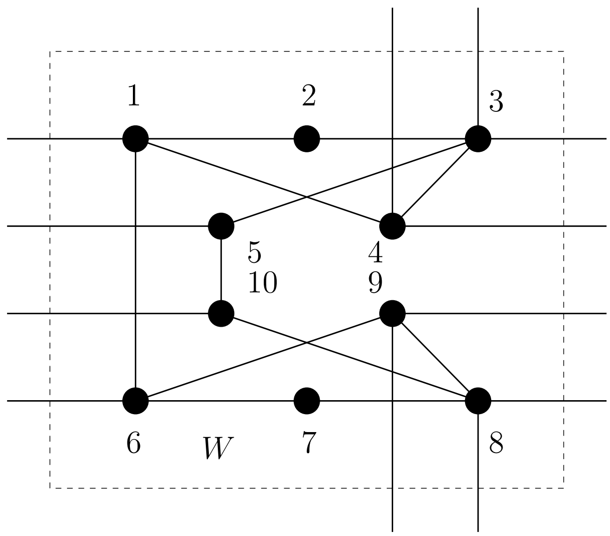

Figure 5. The fundamental domain V of the $\mathbb{Z}^2$-periodic graph Λ.

Figure 5 depicts the fundamental domain of a more symmetric periodic graph.

We now define the Floquet Laplacian $\Delta(k) : \ell^2(V) \to \ell^2(V)$ as the restriction of Δ defined as in (2.1) to the space ℓ^2_k. In terms of the basis of the delta functions at vertices of V, this operator has the following matrix:

$$\Delta(k) := \begin{pmatrix} A & B \\ B^\dagger & A \end{pmatrix}, \tag{2.10}$$

where A is the matrix

$$A(k) := \begin{pmatrix} 0 & 1 & \mathrm{e}^{-\mathrm{i}k_1} & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ \mathrm{e}^{\mathrm{i}k_1} & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & \mathrm{e}^{\mathrm{i}k_1} \\ 0 & 0 & 1 & \mathrm{e}^{-\mathrm{i}k_1} & 0 \end{pmatrix}, \tag{2.11}$$

and B is

$$B(k) := \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}k_2} & 0 & 0 \\ 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}k_2} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{2.12}$$

The matrix B describes the interaction between the two symmetric halves of the fundamental domain V.

In a similar way, one can define $L(k)$ and observe that

$$L(k) = \begin{pmatrix} T^{-1} & 0 \\ 0 & T^{-1} \end{pmatrix} \Delta(k) \begin{pmatrix} T^{-1} & 0 \\ 0 & T^{-1} \end{pmatrix}, \tag{2.13}$$

where T is the matrix

$$T := \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{5} & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{3} \end{pmatrix}. \tag{2.14}$$

The fundamental domain has 10 vertices, and so there are 10 bands to the spectrum. The lowest 5 bands are approximately $[-3.840, -2.265]$, $[-2.943, -1.834]$ $[-1.865, -1.113]$, $[-1.536, -0.333]$ and $[-0.803, 0.377]$. The spectrum is symmetric about $\lambda = 0$, and the remaining five bands are reflections of the previously mentioned bands about this point.

We again focus on a single example: the third band $[-1.865, -1.113]$. A greyscale plot of the reduced Brillouin zone‖ for the solution curve corresponding to this band is given in Figure 6. On the other hand, Figure 7 represents the band $[-2.943, -1.834]$, for which maxima and minima occur both on the boundary Ξ of the reduced Brillouin zone (albeit, not on X). For the graph Λ we have observed that only the lower edge of the third band, and upper edge of the eighth band are away from the boundary of the reduced Brillouin zone. All other band edges do occur on these lines of symmetry of the Brillouin zone.

In order to check that the minimum point of the third branch really occurs away from the boundary of the reduced Brillouin zone, we repeat the procedure described in Section 2.1. With the aid of symbolic algebra computer packages such as `Maple` it is easy to find the characteristic polynomial of the 10×10 matrix (2.10), and to compute the derivative along the lines $k_1, k_2 = 0, \pi$. This leads to a set of four pairs of polynomial equations (in the variables λ and $\cos(k_1)$ (or $\cos(k_2)$)) to be solved simultaneously. Numerical root finding of this system reveals the minimum along the boundary to occur at the point $k \approx (1.970, 0)$ attaining a minimum value $\lambda \approx -1.830$. We compare this

‖ Note that for this figure, the *reduced* Brillouin zone $[0, \pi]^2$ is plotted. The picture for the full Brillouin zone is obtained by reflection of this picture in 2 directions.

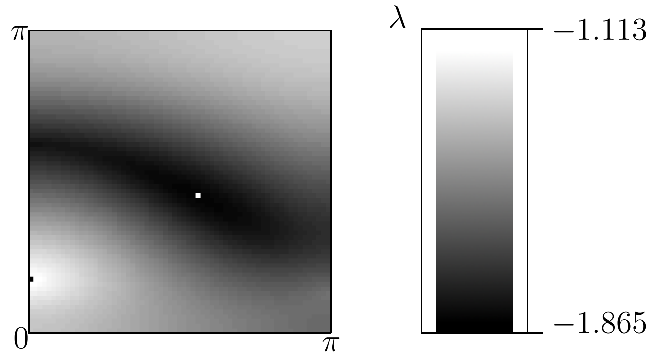

Figure 6. A gray scale image of the third branch of the spectrum of $\Delta(k)$. Extreme points are highlighted.

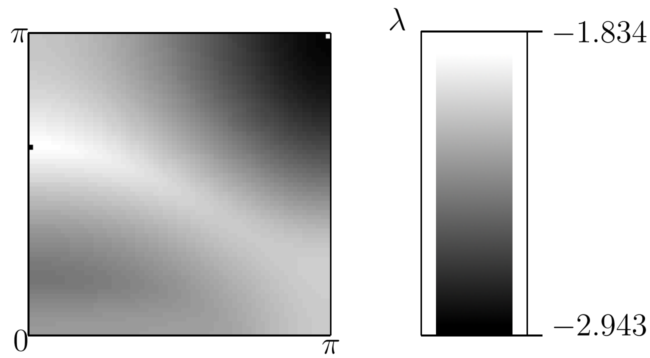

Figure 7. A gray scale image of the second branch of the spectrum of $\Delta(k)$. Extreme points are highlighted.

with the strictly lower point in the interior at $k \approx (1.41, 1.78)$ which takes the value $\lambda \approx -1.865$, a difference of approximately 2% (or 5% of the width of the band).

Looking only at the four "corner" points: $(0, 0)$, $(0, \pi)$, $(\pi, 0)$, (π, π), the minimum value attained on the third band is $\lambda \approx -1.568$.

For the operator $L(k)$ the situation is qualitatively similar. The positions of the various maxima and minima do not move much. The minimum of the third band is located again away from the boundary of the Brillouin zone. At the point $k \approx (1.28, 1.93)$ the value attained by the third band function is $\lambda \approx -0.5486$. It turns out that the minimum value taken on the boundary of the reduced Brillouin zone is $\lambda \approx -0.5380$ at $k \approx (1.92, 0)$, a difference of 2% (or 6% of the width of the band).

One can also notice that we encounter here examples of spectral edges occurring on Ξ, but not on X. So, all the possibilities do materialize: spectral edges occurring on X only, on $\Xi - X$, and finally on $B - \Xi$.

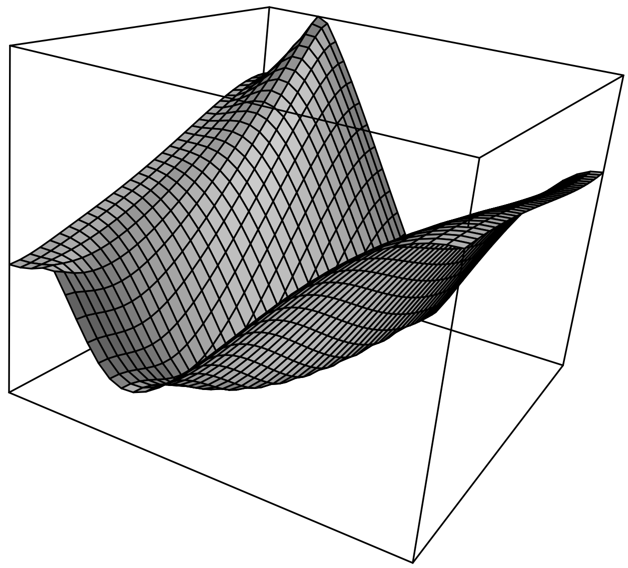

Figure 8. A graph of the third branch.

3. Quantum graph case

In this section we consider the spectrum of a periodic quantum graph G with the same topology as Γ. The spectrum $\sigma(G)$ can be related to the spectrum of the Floquet Laplacian $L(k)$ investigated in the previous section. As a consequence, we will discover that the maxima and minima of some branches, and thus spectral edges as well, occur at the same quasi-momenta in both systems. Hence, spectral edges of this periodic quantum graph Hamiltonian occur inside the Brillouin zone.

We construct a metric graph G by equipping all edges of Γ with unit lengths. To complete the definition of a quantum graph, we need to define a self-adjoint differential Hamiltonian. As such, we consider the negative second derivative on the edges e of G:

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x_e^2}\ . \tag{3.15}$$

The Hilbert space where the operator acts is $L^2(G) = \bigoplus_e L^2(e)$. The domain of

the operator consists of all functions f such that

$$\begin{cases} f \in H^2(e) \text{ for each edge } e, \\ \sum_e \|f\|^2_{H^2(e)} < \infty, \\ f \text{ is continuous at each vertex} \\ \sum_{e\sim v} f'_e(v) = 0 \text{ (Kirchhoff, or Neumann, conditions).} \end{cases} \tag{3.16}$$

Here, $f'_e(v)$ denotes the outgoing derivative of f at v along the edge e.

It is well known (e.g., [16, 40, 43, 49]) and easy to check that Floquet theory applies to the quantum graph case. In particular, the spectrum $\sigma(H)$ coincides with the union over the Brillouin zone B of the spectra of Floquet Hamiltonians $H(k)$. Here $H(k)$ is the operator defined similarly to H on H^2_{loc} functions with the same Kirchhoff vertex conditions as in (3.16), and with the additional cyclic (Bloch, Floquet) condition (2.3):

$$f(T(px)) = \mathrm{e}^{\mathrm{i}k\cdot p} f(x) \tag{3.17}$$

for any $p \in \mathbb{Z}^2$, $x \in G$. We will call such functions *Bloch (generalized) eigenfunctions*. Thus, describing the spectrum of an either combinatorial, or quantum periodic graph operator, we can work with such generalized eigenfunctions only.

So, let ψ be a Bloch eigenfunction of H on G with a quasimomentum k and eigenvalue ω^2,

$$H\psi = \omega^2\psi\ . \tag{3.18}$$

Let us define a function φ on the combinatorial counterpart Γ of G as the restriction of ψ to the vertices of G. Clearly, φ is a Bloch function with the same quasimomentum k (e.g., [40]). Due to (3.18), on each edge $e = (u, v)$ the function ψ can be written in terms of its values $\varphi(v), \varphi(u)$ at the endpoints:

$$\psi_e(x_e) = \varphi(v)\cos\omega x_e + \left(\frac{\varphi(u) - \cos\omega\,\varphi(v)}{\sin\omega}\right)\sin\omega x_e \tag{3.19}$$

Here ψ_e and x_e denote the restriction of ψ to the edge e and the coordinate along e respectively. Then one has

$$\psi'_e(v) = \frac{\varphi(u) - \cos\omega\,\varphi(v)}{\tan\omega}. \tag{3.20}$$

Vertex conditions (3.16) imply that at each vertex v the equation

$$\frac{1}{d_v}\sum_{u\sim v}\varphi(u) = \cos\omega\,\varphi(v) \tag{3.21}$$

holds. Thus, φ is a Bloch eigenfunction of the difference operator $\frac{1}{d_v}\sum_{u\sim v}\varphi(u)$ on Γ with eigenvalue $\cos\omega$. Notice that the spectrum of this operator coincides with the spectrum of its symmetrized version L investigated in the previous section. Thus, we have constructed a quantum graph example of a periodic operator with a spectral edge attained inside the Brillouin zone.

The reader might notice that the correspondence between the spectra of L and H works smoothly only outside zeros of $\sin \omega$, i.e. not on the Dirichlet spectrum of the edges. This is a well known phenomenon, see for instance [40]. However, it is easy to observe that this does not influence our case and thus we have an example when a spectral edge of a periodic quantum graph occurs inside the Brillouin zone.

4. Neumann waveguides and periodic tubular manifolds

In this section, we will show existence of periodic elliptic second order operators on manifolds with a free co-compact action of $\mathbb{Z}^2$, some of whose spectral edges are attained inside the Brillouin zone. The simplest example is of the Laplace operator with Neumann boundary conditions in a periodic planar waveguide.

In order to construct the guide, let us assume our graph G (see Figure 1) to be embedded into the plane in such a way that:
1. Each edge is a smooth simple curve of length 1.
2. Edges intersect only at the vertices.
3. Edges intersect transversally (i.e., there are no tangent edges).
4. The embedded graph is $\mathbb{Z}^2$-periodic.

Such an embedding is clearly possible.

Let us take a small $\varepsilon > 0$ and consider a "fattened graph" domain Ω_ε that consists of tubular neighborhoods of the edges (domain U in Figure 9 below) and neighborhoods of vertices (domain V in Figure 9).

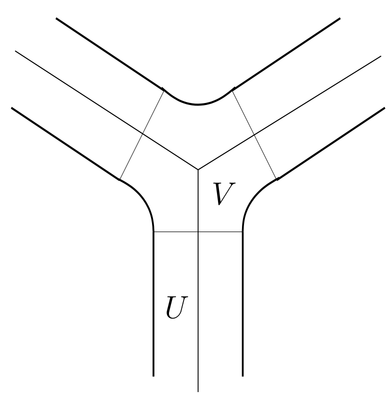

Figure 9. A "fattened graph" domain.

We will assume the following conditions on the domain Ω_ε:
1. The boundary is sufficiently smooth (e.g., C^2).
2. The domains U have constant width ε in directions normal to the edges.
3. The vertex neighborhoods V satisfy the following property: there exist balls b_ε and B_ε of radii $r\varepsilon$ and $R\varepsilon$ correspondingly, centered at each vertex and such that $b_\varepsilon \subset V \subset B_\varepsilon$. Besides, V must be star-shaped with respect to all points of b_ε.
4. The domain Ω_ε is $\mathbb{Z}^2$-periodic.

It is easy to see that one can construct an ε-dependent family of domains satisfying all these properties.

Consider now the (positive) Laplace operator $-\Delta_{N,\varepsilon}$ in Ω_ε with Neumann boundary conditions on $\partial\Omega_\varepsilon$.

It is proven in [44, 45], [54]-[57] that for any value of the quasimomentum k and any finite interval I of the spectral axis, the part in I of the spectrum of the Floquet operator $-\Delta_{N,\varepsilon}(k)$ converges to the corresponding part of the spectrum of the quantum graph Hamiltonian (3.15)-(3.16) on G. Moreover, this convergence is uniform with respect to k. This, in particular, implies immediately the following

Theorem 4.1. *For sufficiently small values of ε, there is an isolated band of the spectrum of the waveguide operator $-\Delta_{N,\varepsilon}$, whose end points are attained strictly inside the first Brillouin zone.*

Proof. Indeed, this property holds for the quantum graph Hamiltonian H on G, and thus the convergence result shows that it survives in Ω_ε for small values of ε. □

This construction does not necessarily require the graph to be planar. For instance, one would not be able to have a planar embedding with required properties for the more symmetric graph Λ considered in Section 2.3. However, one can embed Λ into $\mathbb{R}^3$ in such a way that it is $\mathbb{Z}^2$-periodic, with all other properties as required before. Then a $3D$ waveguide domain Ω_ε can be constructed around Λ in a similar manner to the one above, such that the statement of Theorem 4.1 still holds.

Another type of examples can be constructed as a "tight sleeve Riemannian manifold" M_ε around graphs G or Λ. The notion of such a manifold can be easily understood from the Figure 10 (see precise definitions in [17]).

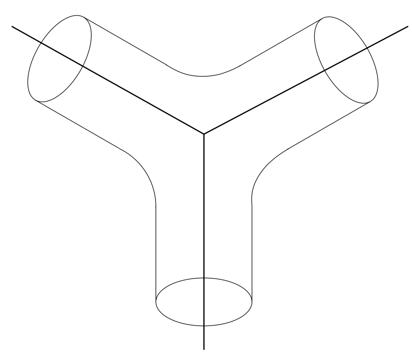

Figure 10. A "sleeve" manifold.

Such a manifold can be constructed preserving a co-compact free action of $\mathbb{Z}^2$. Then the results of [17] concerning convergence of spectra of the Laplace-Beltrami operator on M_ε to those on the graph, show that the following result holds:

Theorem 4.2. *In any dimension $d \geqslant 2$, there exists an example of a closed d-dimensional manifold M with a co-compact, free, isometric action of $\mathbb{Z}^2$, such that there is an isolated band of the spectrum of the Laplace-Beltrami operator $-\Delta_M$, whose end points are attained strictly inside the first Brillouin zone.*

The proof coincides with the one of the previous theorem.

5. Schrödinger and Maxwell operators

The previous discussion does not leave any doubt that examples can be found for essentially any type of periodic equations of mathematical physics. However, it is desirable to have such explicitly described examples for the cases of periodic Schrödinger and Maxwell equations, interest in which stems from the solid state and photonic crystal theories (e.g., [1], [19]-[21], [30, 31], [35]-[37], [53]).

Although we do not currently have rigorous arguments to show the existence of such examples, we can expect that they may be obtained as follows. Consider a planar embedding of the graph G, as the one considered in the previous section, with the additional requirement that at each vertex the tangent lines to the converging edges form equal angles. This can obviously be achieved. Consider then a "fattened graph" domain Ω_ε described before and the Schrödinger operator $S := -\Delta + V(x)$ in $\mathbb{R}^2$ with the $\mathbb{Z}^2$-periodic potential $V(x)$ that is equal to zero in Ω_ε and equal to a large constant C outside.

Conjecture 5.1. *Under appropriate asymptotics $\varepsilon \to 0, C \to \infty$, the spectrum of the operator S will display an isolated spectral band with its edges attained inside the Brillouin zone.*

What is lacking here, in spite of significant attention paid to such asymptotics (e.g., [11, 12, 15, 17, 18, 22, 23, 25, 36, 37, 38, 41, 42, 44, 45, 46, 47, 52], [54]-[59], [63]), is a spectral convergence result analogous to the one for the Neumann Laplace operator. Moreover, it is known that such convergence (even after appropriate spectral re-scaling), does not hold, due to the appearance of low energy (below the energy of the first transversal eigenfunction) bound states attached to vertices [12, 18, 38]. However, for creating an example that we are looking for, the full spectral convergence is not truly needed. What is required, is some kind of convergence above the energy of the first transversal eigenfunction, which must hold (see some results in this direction in [46, 47]). When the angles formed by the edges are equal, we expect vertex conditions of Kirchhoff type to arise.

Concerning the periodic Maxwell operators $\nabla\times\varepsilon^{-1}(x)\nabla\times$, where $\varepsilon(x)$ is the electric permeability, we expect that the simplest to come by will be an example of a $2D$ periodic medium (i.e., a medium which is periodic in two directions and homogeneous in the third one). As it is well known [29, 30, 31, 37], in this case the Maxwell operator splits (according to two polarizations) into the direct sum of two scalar operators $-\nabla\cdot\varepsilon^{-1}(x)\nabla$ and $-\varepsilon^{-1}(x)\Delta$. We expect that similar high-contrast narrow media as described above should provide necessary examples (see also considerations of such high contrast limits in [3], [19]-[21],[24, 28, 37, 41, 42, 60]).

6. Why do spectral edges often appear at the symmetric points of the Brillouin zone?

In this section, we will show why, in spite of the examples of this paper, the spectral edges are often attained at the highest symmetry points, and hence at the boundary of the reduced Brillouin zone. Namely, let H_0 be a periodic self-adjoint elliptic Hamiltonian with real coefficients (i.e., the corresponding non-stationary Schrödinger equation has time-reversal symmetry). Suppose that the spectral edges of H_0 are attained at symmetry points of the Brillouin zone $B = [-\pi, \pi]^n$ only (see the details below). Then we will show that for a "generic" H_0, this feature of the spectrum cannot be destroyed by small perturbations (with the same symmetry) of the operator. This robustness might be the reason why one very rarely observes spectral edges appearing inside the reduced Brillouin zone.

Let us now introduce some notions. We will assume, for simplicity of presentation, that the Hamiltonian is the Schrödinger operator in $\mathbb{R}^n$:

$$H_0 = -\Delta + V(x), \tag{6.22}$$

where $V(x)$ is a real-valued bounded potential such that $V(x+p) = V(x)$ for all integer vectors $p \in \mathbb{Z}^n$. For any quasimomentum $k \in B$, we will denote by $H(k)$ the Bloch Hamiltonian defined on $\mathbb{Z}^n$-periodic functions (i.e., on functions on the torus $\mathbb{T}^n = \mathbb{R}^n/\mathbb{Z}^n$) as

$$H(k) = \left(\frac{1}{\mathrm{i}}\nabla + k\right)^2 + V(x).$$

It depends polynomially, and thus analytically, on k. We denote by $\lambda_j(k), j = 1, 2, \dots,$ the eigenvalues of $H(k)$ counted with their multiplicity in non-decreasing order. The band functions $\lambda_j(\,\cdot\,)$ are continuous functions of $k \in B$. Since the potential V is real-valued, the eigenvalues are also even in k, i.e. $\lambda_j(-k) = \lambda_j(k)$. This follows from the fact that complex conjugate to an eigenfunction is an eigenfunction (presence of a magnetic potential would destroy this symmetry). This symmetry will be crucial for what follows.

The ranges

$$\Delta_j = \{\lambda_j(k) |\, k \in B\}$$

are closed finite intervals of the spectral axis (*spectral bands*), whose union is the spectrum $\sigma(H_0)$. Global maxima and minima of the band functions $\lambda_j(\,\cdot\,)$ are the endpoints (edges) of spectral bands. It is also known (e.g., [32, 35, 53]) that λ_j's are analytic in k away from the eigenvalue crossing points. In case of the crossing, we point out the following elementary, but useful result:

Lemma 6.1. *Let us fix an open interval $\Delta = (a, b) \subset \mathbb{R}$. Suppose that for a neighborhood $U \subset B$ the band functions λ_s, $j \leqslant s \leqslant j + m$, satisfy*

$$\lambda_s(k) \in \Delta,\ \ k \in U,$$

and that the remaining band functions take values in U that lie outside a neighborhood of the closed interval $\overline{\Delta}$. Then the functions

$$\prod_{s=j}^{j+m} \lambda_s(k) \text{ and } \sum_{s=j}^{j+m} \lambda_s(k) \tag{6.23}$$

are analytic with respect to $k \in U$.

Proof. Let us assume that $m = 1$ (the case of arbitrary m works out exactly same way), i.e. we have two eigenvalue branches $\lambda_-(k) := \lambda_j(k)$ and $\lambda_+(k) := \lambda_{j+1}(k)$. Consider a positively oriented circle $\Gamma \subset \mathbb{C}$ centered at $(a+b)/2$ with radius $(b-a)/2 + \varepsilon$ with a small $\varepsilon > 0$. The two-dimensional projection

$$P(k) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma (\lambda - H(k))^{-1}\, d\lambda, \tag{6.24}$$

depends analytically on $k \in U$. Let $M(k)$ be the range of $P(k)$. It forms an analytic two-dimensional vector-bundle [35, 62]. Let $\{e_1, e_2\}$ be a basis in $M(k_0)$ with some $k_0 \in U$. For k close to k_0 we can define a basis of $M(k)$ analytically depending on k as follows:

$$f_j(k) := P(k)e_j. \tag{6.25}$$

In this basis, the operator function

$$P(k)H(k)P(k)|_{M(k)} = H(k)P(k)|_{M(k)}$$

can be written as an analytic 2×2 matrix-function $A(k)$ with eigenvalue branches $\lambda_-(k)$ and $\lambda_+(k)$. Therefore, the functions

$$\det A(k), \quad \operatorname{tr} A(k)$$

are analytic in k in a neighborhood of k_0. □

The only fixed points $k \in B$ for the symmetries $k \to -k + p, p \in 2\pi\mathbb{Z}^n$, are the ones from the set

$$X = \{k = (k_1, \cdots, k_n) \in B \,|\, k_j \in \{0, \pi\}, j = 1, \cdots, n\}. \tag{6.26}$$

In view of the symmetry $\lambda_j(k) = \lambda_j(-k)$ we also have $\lambda_j(k_0 + k) = \lambda_j(k_0 - k)$ for any $k_0 \in X$. We have already shown in this text that the global extrema of the band functions can occur outside the set X. The experimental observation, however, is that for most periodic operators of practical importance and for practical values of their parameters (e.g., potentials, electric permittivity, etc.), the band endpoints do occur on X. One can easily observe this by looking at dispersion curve calculations in solid state physics or photonic crystals literature (e.g., [51, ?]). **Our main question now is: Why do the spectral edges occur so often on X?**

Our considerations will be local on the spectrum. Thus, let us fix a finite interval $\Lambda = (a, b)$ of the spectral axis. Note that the number of spectral bands Δ_j overlapping with Λ is finite. We first introduce the following notion:

Definition 6.2. *We call a periodic Hamiltonian H* **simple** *on a finite interval Λ, if the global extrema of the band functions $\lambda_j(k)$ which occur inside Λ, are attained at the points of the set X only.*

The simplicity property defined above will be discussed for "generic" periodic operators:

Definition 6.3. *We call a periodic Hamiltonian H* **generic** *on a finite interval Λ, if for every band edge λ_0 occuring inside Λ, the band functions λ_j assume the value λ_0 at finitely many points of the Brillouin zone B, and in a neighborhood U of each such point k_0 one of the following two conditions is satisfied:*

(i) There is a unique band function $\lambda(\ \cdot\ )$ for $k \in U$ such that $\lambda(k_0) = \lambda_0$; moreover, k_0 is a non-degenerate extremum of $\lambda(k)$.

(ii) For $k \in U$ there are only two band functions $\lambda_+(\ \cdot\ )$, $\lambda_-(\cdot\ )$ such that $\lambda_-(k_0) = \lambda_+(k_0) = \lambda_0$. Moreover, $\lambda_-(k) < \lambda_+(k)$ for all $k \in U - \{k_0\}$, and k_0 is a non-degenerate maximum of the product $D(k) = (\lambda_+(k) - \lambda_0)(\lambda_-(k) - \lambda_0)$.

Above by a non-degenerate extremum we understand an extremum with a non-degenerate Hessian.

Recall that in view of Lemma 6.1, the determinant of $A(k)$ is analytic on U. Definition 6.3 means that the band functions of a generic Hamiltonian behave near band edges as eigenvalues of a "generic" 2×2 self-adjoint analytic matrix function. We refer to cases (1) and (2) in the above definition as *the single edge case* and *the case of two touching bands* respectively. Note also that in Definition 6.3 the band edge λ_0 is not assumed to be (albeit could be) an endpoint of the spectrum.

The following conjecture is believed to hold (see a variety of similar genericity conjectures in, e.g., [2, 8, 37, 48]).

Conjecture 6.4. *Generic periodic Hamiltonians form a set of second Baire category in a suitable class of periodic operators.*

The closest to the proof of this conjecture is the result of [33], where it was shown that generically a band edge, which is an endpoint of the spectrum, is attained by a single band function.

Our aim is to show that a generic simple Hamiltonian H_0 remains generic and simple under small perturbations. More precisely, we introduce the family of operators

$$H_g = H_0 + gV(x),\ H_0 = -\Delta + V_0,$$

where V_0 and V are bounded real-valued $\mathbb{Z}^n$-periodic functions, and $g \in \mathbb{R}$ is a parameter. We denote by $\lambda_j(k, g)$ the band functions of H_g. If $g = 0$, we drop g and write simply $\lambda_j(k)$. Since H_g is analytic in g, the band functions $\lambda_j(k, g)$ are analytic in (k, g) away from the crossing points, and the quantities defined in (6.23) are analytic in (k, g) under the conditions of Lemma 6.1.

We can now formulate a result that gives a partial answer to the question posed in this Section.

Theorem 6.5. *Let $\Lambda \subset \mathbb{R}$ be a finite closed interval, and let the operator H_0 (see (6.22)) be simple and generic in a neighborhood of Λ. Then, for sufficiently small values of g, the operator H_g is also simple and generic in a neighborhood of Λ.*

Proof. Let Λ' be a finite closed interval containing Λ in its interior and such that operator H_0 is simple and generic in an open neighborhood Λ'' of Λ'. The continuity of $\lambda_j(k,g)$ in g guarantees that for small g, the spectral band edges of the perturbed operator occurring on Λ', are either perturbations of the band edges of H_0 that are inside Λ'', or are produced by opening a gap between two touching spectral bands of H_0.

Let $\lambda_0 \in \Lambda''$ be a single band edge of H_0, or the point where two bands touch. Assume without loss of generality that $\lambda_0 = 0$. Since the unperturbed operator H_0 is simple, again, by continuity of $\lambda_j(k,g)$ in g, for sufficiently small values of g, the perturbed eigenvalues cannot reach their global maxima outside a neighborhood of the set X. Thus, it suffices to consider the neighborhood of each point $k_0 \in X$ individually. We assume without loss of generality that $k_0 = 0$.

Further proof requires different arguments for the two cases featuring in Definition 6.3.

6.1. The single edge case

Let $\lambda(k)$ be the unique band function of the operator H_0, which attains at $k_0 = 0$ its non-degenerate extremum, which for definiteness will be assumed to be a maximum. Recall that $\lambda(\,\cdot\,)$ is analytic in k and $\lambda(k) = \lambda(-k)$, so that

$$\lambda(k) = \lambda_2(k) + \lambda_e(k),$$

where λ_2 is a negative definite quadratic form and λ_e is an analytic function such that $\lambda_e(k) = \mathrm{O}(|k|^4)$. For sufficiently small g and k, the eigenvalue $\lambda(k,g)$ will remain separated from the rest of the spectrum of $H_g(k)$. Thus, to complete the proof, we need to show that $\lambda(\,\cdot\,,g)$ attains its maximal value at $k = 0$ and this maximum is non-degenerate. Due to analyticity,

$$\lambda(k,g) = \lambda_2(k) + \lambda_e(k) + g\widetilde{\lambda}(k,g),$$

where $\widetilde{\lambda}(k,g)$ is a real-valued real-analytic function of (k,g), and $\widetilde{\lambda}(k,g) = \widetilde{\lambda}(-k,g)$. The latter property implies that

$$\nabla_k\widetilde{\lambda}(k,g) = \mathrm{O}(|k|),$$

uniformly in g. Making an appropriate linear change of variables, we can always assume that $\lambda_2(k) = -|k|^2/2$. Then, taking the gradient with respect to k, we obtain

$$\nabla_k\lambda(k,g) = -k + \nabla_k\lambda_e(k) + g\nabla_k\widetilde{\lambda}(k,g).$$

Consequently

$$|\nabla_k\lambda_e(k) + g\nabla_k\widetilde{\lambda}(k,g)| \leqslant C(|k|^3 + g|k|),$$

with some positive constant C, and hence, for $|g| < (4C)^{-1}, |k| < (2\sqrt{C})^{-1}, k \neq 0$, we get,

$$|\nabla_k \lambda(k,g)| > \frac{|k|}{2} \neq 0.$$

This proves that the only stationary point of $\lambda(\,\cdot\,, g)$ is $k=0$. Moreover, since $\lambda_2(\,\cdot\,)$ is negative definite, the function $\lambda(\,\cdot\,, g)$ has a non-degenerate Hessian if g is sufficiently small. Thus the band function $\lambda(k,g)$ attains its extremum on X and satisfies the requirements of Definition 6.3(1).

6.2. The case of two touching bands

Assume, as above, that $\lambda_0 = 0$, $k_0 = 0$, and that $\lambda_-(k)$ and $\lambda_+(k)$ are the band functions as given in Definition 6.3. Denote by $\lambda_\pm(k,g)$ the perturbed band functions. According to Lemma 6.1, the functions

$$d(k,g) = \lambda_-(k,g)\lambda_+(k,g),\ t(k,g) = \frac{1}{2}(\lambda_-(k,g) + \lambda_+(k,g))$$

are analytic in a neighborhood of $(k,g) = (0,0)$. Remembering the central symmetry of the eigenvalues and the genericity assumption for H_0, we can write

$$\begin{aligned} d(k,g) &= d_2(k) + d_e(k) + g\widehat{d}(k,g), \\ t(k,g) &= t_2(k) + t_e(k) + g\widehat{t}(k,g). \end{aligned} \tag{6.27}$$

Here all functions are analytic near $(k,g) = (0,0)$ and even in k. The functions t_2 and d_2 are quadratic forms, the terms d_e, t_e are $\mathrm{O}(|k|^4)$, and, by virtue of genericity, d_2 is negative definite. Thus, as in the first part of the proof, we may assume that $d_2(k) = -|k|^2/2$. Note also, that $\hat{d}(0,g) = 0$, since the eigenvalues $\lambda_\pm(0,g)$ are of order $\mathrm{O}(g)$, and hence $d(0,g) = \mathrm{O}(g^2)$. Introduce the quantity

$$m = t^2 - d = \frac{1}{2}(\lambda_+ - \lambda_-)^2 \geqslant 0.$$

Using (6.27) we get

$$m(k,g) = g^2 m_0(g) - d_2(k) + m_e(k,g),\ m_e(k,g) = \mathrm{O}(|k|^2)(k^2 + g),$$

where the functions $m_0(g) = \hat{t}(0,g)^2 - \partial_g \hat{d}(0,g)$ and $m_e(k,g)$ are analytic in k, g, and m_e is even in k. Since $m(0,g) = g^2 m_0(g)$, we also have $m_0(g) \geqslant 0$.

Let us list some simple estimates that these functions and their gradients with respect to k satisfy in a neighborhood of $(0,0)$. Below we denote by C, C_1 some positive constants whose precise value is not important:

$$\begin{aligned} &|t(k,g)| \leqslant C(k^2 + g),\ |m(k,g)| \leqslant C(|k|^2 + g^2), \\ &|\nabla_k t(k,g)|, |\nabla_k m(k,g)| \leqslant C|k|, \end{aligned} \tag{6.28}$$

$$\begin{aligned} &|\nabla_k m(k,g)| \geqslant \frac{1}{2}|k|, \\ &m(k,g) \geqslant g^2 m_0(g) + \frac{1}{4}|k|^2. \end{aligned} \tag{6.29}$$

The eigenvalues $\lambda_\pm(k,g)$ solve the characteristic equation

$$\lambda^2 - 2t(k,g)\lambda + d(k,g) = 0,$$

and thus

$$\lambda_\pm(k,g) = t(k,g) \pm \sqrt{m(k,g)}. \tag{6.30}$$

By (6.29) the eigenvalues $\lambda_\pm(k,g)$ can coincide only at $k=0$, so that they are analytic in k for $k \neq 0$. Let us prove that $\lambda_\pm(\,\cdot\,,g)$ have no stationary points if $k \neq 0$. Differentiate:

$$\nabla_k \lambda_\pm(k,g) = \nabla_k t(k,g) \pm \frac{\nabla_k m(k,g)}{2\sqrt{m(k,g)}}.$$

Now the estimates (6.28) and (6.29) imply:

$$|\nabla_k \lambda_\pm| \geqslant \left|\frac{\nabla_k m}{2\sqrt{m}}\right| - |\nabla_k t| \geqslant \frac{c|k|}{\sqrt{|k|^2+g^2}} - C|k| \geqslant C_1|k|$$

for small g and $k \neq 0$. This proves that $\lambda_\pm(\,\cdot\,,g)$ attain their extrema only at $k=0$.

It remains to show that the eigenvalues satisfy the requirements either of Part (1) or Part (2) of Definition 6.3. If $m_0(g) > 0$, then by (6.29) and (6.30), the eigenvalues $\lambda_+(k,g)$ and $\lambda_-(k,g)$ are decoupled for all k and g, and their extrema are clearly non-degenerate. If $m_0(g) = 0$, then by (6.30) $\lambda_+(0,g) = \lambda_-(0,g)$, and then by (6.27) the determinant $d(k,g)$ has a non-degenerate Hessian for small k, g.

The proof of the 6.5 is complete. □

7. Final remarks

- Suppose that for a particular periodic operator the spectral edges do occur at the point of $X = \{k|\, k_j = \pm\pi \text{ or } 0\}$ only. This means then that one can find the correct spectral edges (and thus the spectrum as a set), computing only spectra of problems that are periodic or anti-periodic with respect to each variable (say, periodic with respect to x_1 and x_3 and anti-periodic with respect to x_2). This resembles then the $1D$ situation [13, 53], when the edges of the spectrum are attained at the spectra of the periodic and anti-periodic problems.
- In the last Section we have restricted ourselves to the case of Schrödinger operators with electric potentials only. However, the proof in fact does not use the structure of the operator and could be extended to arbitrary analytically fibered operator in the sense of [26], as long as the central symmetry $k \mapsto -k$ holds.
  We also assumed parametric perturbation (i.e., perturbation by gV with a small scalar parameter g). However, without any change in the proof, one can consider V as a functional parameter and prove the same statements for small values of this parameter.
- Observations of stability under small perturbations of critical points of a function in "general position" in presence of symmetries, analogous to the ones in the last section, have been made before in different circumstances, e.g. in [27].

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